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Effect of Boron Speciation on Diffusivity, Compressibility, and Mechanics of Borosilicate Glasses

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Boric oxide (B_2O_3) is widely used as a network forming constituent in many high-tech glass materials owing to its contribution to high glass forming ability and low melting temperature, and for its favorable impact on thermal, mechanical, and optical properties. Boron exhibits dramatic structural changes as a function of chemical composition, pressure, and thermal history in B_2O_3 containing glasses, most notably the conversion among three-fold (B^{III}) and four-fold coordinated boron (B^{IV}). Here we derive a simple two-state statistical mechanical model that can accurately predict the composition and thermal history dependence of the boron speciation, i.e., the relative fractions of B^{III} and B^{IV} . Such prediction is important as we also demonstrate how the two different coordination environments of boron have significantly different effects on, e.g., alkali diffusivity, network compressibility, and crack resistance in borosilicate glasses. We show that B^{III} is associated with a more open and compliant structure, favoring fast alkali diffusivity and network densification, which in turn improves the crack resistance. Our findings thus have important implications for the rational design of damage resistant glasses.

Keywords: boron; network structure; borosilicate glass